Combustion Simulation Databases for Real Transportation Fuels

US transportation is powered by fossil fuels, with a fuel cost of over $500 billion/year. Efficiency of diesel, gasoline, and aviation engines directly affects the economy, and emissions of CO_2 and other pollutants have significant implications with respect to climate change, health care costs, and the environment. Accurate combustion-models are needed to enable advanced computer based strategies for the design of more efficient and less polluting engines, and engines that take advantage of alternate (secure) fuels. At present the physical and chemical data necessary to develop these combustion models are not available. A NIST-sponsored workshop held in 2003 and involving industrial, academic, and governmental stakeholders identified developments necessary to address the technical barriers and measurement needs. Widely expressed was a desire for NIST to play a leadership role in meeting the physical and chemical properties data needs and to aid in the development of a standard infrastructure for the exchange of combustion related information.

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NIST is working with a number of existing and developing efforts toward the creation of a collaborative community infrastructure for combustion model development. These include efforts such as the Collaboratory for Multi-Scale Chemical Science (CMCS), a computer science effort comprising five national labs and a number of universities, the Process Informatics Model (PrIMe) collaboration aimed at building detailed chemical kinetic models, and emerging industrial, academic, and governmental collaborations on the development of surrogate fuel mixtures. These mixtures are needed to address the complexity of real fuels and enable coordinated research and modeling efforts. Working from the identified surrogates and established data gaps, targeted data evaluations and experimental measurements also are developed by NIST.

As part of NIST data infrastructure efforts, we have created updated XML schema for the data needed by PrIMe to generate chemical kinetic models. NIST has additionally provided ≈75,000 kinetic records of elementary reactions to populate the PrIMe Library and developed software for data input. NIST has developed a preliminary *Detailed Chemical Kinetic Combustion Model Database* (http://kinetics.nist.gov/realfuels/db/index.cgi). This database provides a centralized site for model information (a sophisticated, chemically oriented reaction classification and search interface is illustrated in the figures) and im-plements heretofore lacking standards for nomenclature, notation, and traceability. Data evaluation efforts on select chemical systems also continue. For example a butylbenzene Combustion Kinetics Database has just been released and major improvements in modeling the steps of heptane pyrolysis is underway. Parallel experimental efforts at NIST are aimed at filling key data gaps and resolving uncertainties in the models.

The NIST Detailed Chemical Kinetic Combustion Model Database now includes the ability to upload models in the form of CHEMKIN files (a community standard), and tools that enable the disparate data formats used within the community to be facilely translated to a NIST standard.
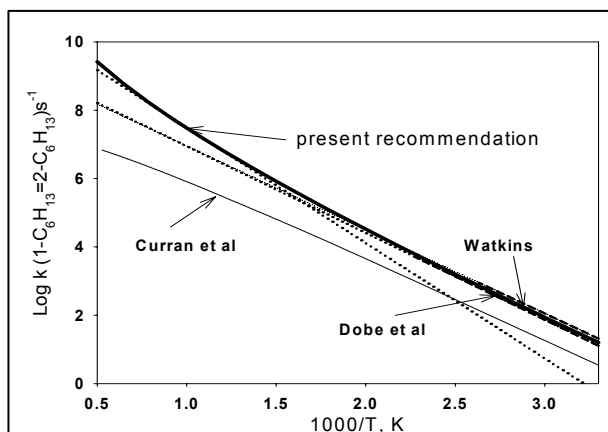
Experimental rate data from the shock tube laboratory are used to fill data gaps and resolve uncertainties in key data in the models. The example above is for the 1-5 isomerization of 1-hexyl radicals.

The emerging infrastructure and standards for the exchange of combustion-related data will overcome one large barrier to progress in the area of combustion processes. This will facilitate coordinated, collaborative research for the design of innovative power systems, thus meeting national needs relating to energy independence, sustainability, climate change, quality of life, and security as well as assuring US engine manufacturers a basis for innovation and international competitiveness.

Future Plans: Functionality of the *Detailed Chemical Kinetic Combustion Model Database* will undergo testing by researchers at universities and national labs in 2006. Software tools to enable greater automation of data input, and the comparison and evaluation of models and data therein, are under development. Enhancing the interoperability of NIST-developed software with other community efforts is also planned. The database efforts are expected to further dovetail with ongoing experimental studies at NIST for mechanisms related to surrogate fuels, and formation of polycyclic aromatic hydrocarbons (PAHs) and soot.

Selected Publications:

- Baulch D.L., Bowman C.T., Cobos C. J., Cox R. A., Just T., Kerr J. A., Pilling, M. J., Stocker D., Troe J., Tsang W., Walker R.W., Warnatz J.; *"Evaluated Kinetic Data for Combustion Modeling"* Supplement II, J. Phys. Chem. Ref. Data. 4 (3): 757-1397, 2005.
- V. I. Babushok and W. Tsang, *"Kinetic Modeling of Heptane Combustion with PAH Formation"*, J. of Propulsion and Power, 20, 403-414, 2004.
- W. Tsang, **"Butylbenzene Combustion Kinetics Database"**, to be published Proceedings of the American Institute of Aeronautics and Astronautics (AIAA) Meeting.

Dynamically linked architecture for reaction information under development for new chemically oriented Chemical Kinetics Model Database.